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**PHASE TRANSITIONS IN THE
ISING MODEL**

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PHASE TRANSITIONS IN THE ISING MODEL

Eva Ellis-Monaghan

Abstract. This paper investigates the Ising model, a model conceived by Ernst Ising to model ferromagnetism. This paper presents a historical analysis of a model which brings together aspects of graph theory, statistical mechanics, and linear algebra. We will illustrate the model and calculate the probability of individual states in the one dimensional case. We will investigate the mathematical relationship between the energy and temperature of the model, and, using the partition function of the probability equation, show that there are no phase transitions in the one dimensional case. We endeavor to restate these proofs with greater clarity and explanation in order for them to be more accessible to other undergraduates.

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1. INTRODUCTION

The Ising model was introduced by Ernst Ising in his doctoral thesis as an attempt to model phase transition behavior in ferromagnets (basic refrigerator magnets)[Isi25], at the suggestion of his thesis advisor, Dr. Wilhelm Lenz. This model is among the simplest statistical mechanical models and bears the distinction of being one of the few to be solved in the two dimensional case. This paper will present a historical analysis of this model and an exposition of the one dimensional solution.

The Ising model is not ideal for ferromagnets although it successfully models a variety of different systems[BEPS10]. However, the conventional terminology developed from the setting of ferromagnetism and therefore a basic understanding of ferromagnets will be useful. A ferromagnet is a material that exhibits spontaneous magnetization. In ferromagnets, magnetic ions in the material align to create a net magnetism or misalign to create a zero net magnetism. Each ion exerts a force on the surrounding ions to align with it. An aligned state is a low energy state, while entropy increases at higher temperatures to cause substantial misalignment. When these individual interactions build to a macro scale, alignment produces a net magnetism.

If there is a sudden change in magnetism at a certain temperature, we say there is a phase transition at that temperature. For instance, if an iron magnet with a net magnetism at 600°C experiences a temperature increase to 900°C , the magnetism will suddenly dissolve at approximately 770°C , the Curie temperature of iron. This is represented mathematically as a failure of analyticity in the energy functions of the magnet.

Although there are phase transitions in higher dimensions, phase transitions do not occur in the one dimensional case of the Ising model. In this paper we will solve the Ising model in one dimension and demonstrate that there are no phase transitions generally following the approaches of Ising[Isi25] and Cibra[Cip87]. The two dimensional model was solved by Onsager[Ons44], and phase transitions are present. The three dimensional model remains unsolved.

2. AN EXPLANATION OF THE MODEL

The Ising model is displayed on a lattice, or a repeating graph. In one dimension, this lattice is a cycle where each vertex is connected to the next, as in Figure 1.

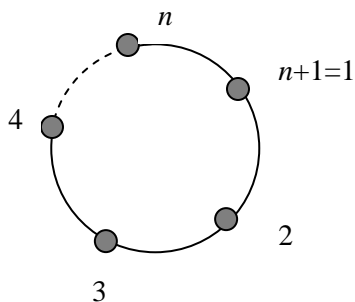


Figure 1

Figure 2 shows the Ising model in two dimensions, displayed on the square lattice. The graph may be wrapped into a torus to avoid boundary conditions.

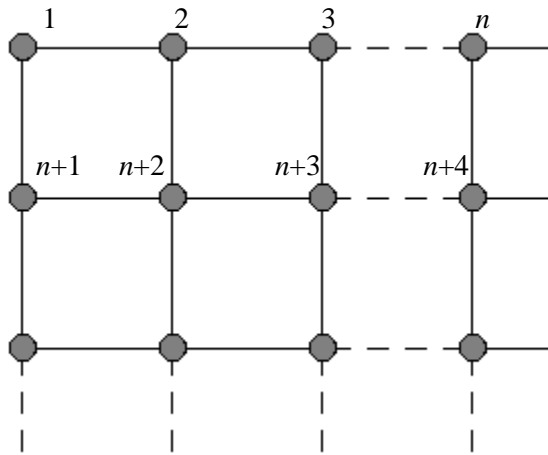


Figure 2

Each vertex is assigned a spin that indicates the direction of the individual ion's magnetism. The spin at each vertex is either up or down. The particular arrangement of spins on a graph is called the state of the graph. Figure 3 shows a state on a $n = 4$ square lattice, where black represents an upward spin, and grey a downward spin.

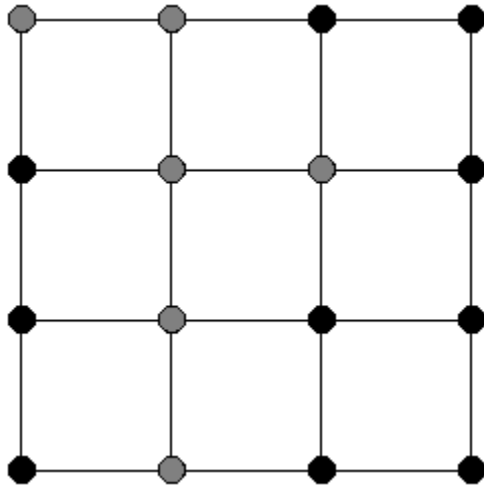


Figure 3

The edges of the graph indicate which vertices are nearest neighbors. For mathematical simplicity rather than scientific accuracy, each vertex is only influenced by its nearest neighbors. A vertex's spin interacts with the spins of its nearest neighbors by exerting a force to align neighboring spins in a lower energy state where all vertices have the same spin as their neighbors. Entropy, measured by temperature, tends to randomize the spins of nearest neighbors. The specific energy of a state is a function of the temperature and the interaction energy between

two spins. In a finite model, this energy corresponds to several possible net magnetisms. As the model grows very large, the magnetism at a specific temperature approaches a single value. We will show that the plot of temperature vs. probability of a net magnetic state of the one-dimensional Ising model is an analytic function as the number of ions approaches infinity.

When the functions of energy or entropy are not analytic, the discontinuity represents a change in physical properties. In ferromagnets, this is a change in net magnetism. Thus the search for phase transitions is synonymous with a search for discontinuities in the functions and their derivatives. Consider for example the phase transition between water and steam. This transition can be crudely modeled with the Ising model, where the vertices are points in space, and the spins, rather than up or down, are the presence or absence of a molecule. Thus the magnetism corresponds to the density of the H₂O. At 100 degrees Celsius, the density changes drastically; a phase transition. A phase transition occurs at a critical, or Curie, temperature.

3. ANALYSIS OF A FINITE ISING MODEL

As the magnetism is related to the free energy in the system, we begin by quantifying the energy of a state of a graph. The Hamiltonian of a state in an Ising model corresponds to the energy of the system. Thus the Hamiltonian is expressed as

$$h(\omega) = -J \sum_{\{i,j\} \in E(G)} \delta(\sigma_i, \sigma_j).$$

Here ω is a state of graph G , and σ_i is the spin at vertex i , while δ is the Kronecker delta function, and J is the interaction energy. The sum is over all edges $\{i,j\}$ in the edge set $E(G)$.

The Hamiltonian sums the number of edge pairings between vertices with the same spins, weighted by the interaction energy. For the Ising model, the Kronecker delta may be defined as the dot product of adjacent spins where each spin is valued as the vector $\langle 1,0 \rangle$ or $\langle 0,1 \rangle$. Thus,

$$h(\omega) = -J \sum_{\{i,j\} \in E(G)} \sigma_i \cdot \sigma_j.$$

This Kronecker delta function is modeled by giving an edge between two like spins a value of 1, and an edge between unlike spins a value of 0. In illustration, consider Figure 4, where an upward spin $\langle 0,1 \rangle$ is represented by a black vertex, and a downward spin $\langle 1,0 \rangle$ is represented by a grey vertex. This state has a Hamiltonian of $-14J$. The lowest energy states, and therefore smallest Hamiltonians, exist where all spins are all in the same direction.

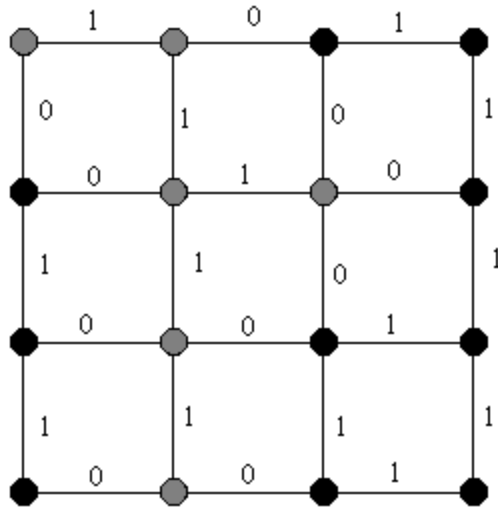


Figure 4

In the Ising model, as in many other forms of statistical models, the probability, $\Pr(\omega, T)$, of a particular state of a graph is a function of the Hamiltonians of all the possible states, and of the temperature T . Higher temperature is related to a higher level of entropy and a more random state, while lower temperature is related to a more ordered state. These probabilities have a Boltzmann distribution:

$$\Pr(\omega, T) = \frac{\exp\left(-\frac{1}{kT} h(\omega)\right)}{\sum_{\text{all } \omega} \exp\left(-\frac{1}{kT} h(\omega)\right)}$$

Here $k = 1.38 \times 10^{-23}$ joules/Kelvin, the Boltzmann constant. This distribution relies on a classical understanding of particles, so it only applies to situations where quantum effects are negligible and it breaks down at temperatures very near absolute zero.

The denominator of the probability function is the same for any state, and is called the partition function Z . The partition function is denoted by:

$$Z = \sum_{\text{all } \omega} \exp\left(-\frac{1}{kT} h(\omega)\right), \text{ which may be rewritten as } Z = \sum_{\text{all } \omega} \prod_{\{i,j\}} \exp\left(\frac{J}{kT} \sigma_i \cdot \sigma_j\right).$$

Example:

To illustrate these concepts more clearly, consider C_4 , the 4-cycle. We will determine all the possible states, identify the partition function, and then calculate the probability of one of these states at several temperatures. All possible arrangements of spins and the Hamiltonians of each state are shown in Figure 5.

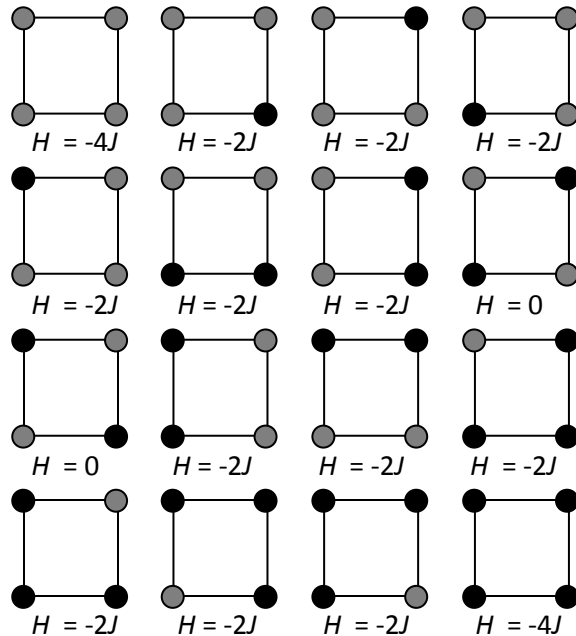


Figure 5

There are two states with a Hamiltonian of $-4J$, two states with a Hamiltonian of 0 , and twelve states with a Hamiltonian of $-2J$. Therefore the partition function for the 4-cycle Ising model is

$$Z = 2 \exp\left(\frac{4J}{kT}\right) + 12 \exp\left(\frac{2J}{kT}\right) + 2.$$

This will be the denominator of our probability calculation. We will calculate the probability of the first state. This state has a Hamiltonian of $-4J$, and is one of the two lowest energy states. The probability of this state occurring is:

$$\Pr(\omega, T) = \frac{\exp\left(\frac{4J}{kT}\right)}{2 \exp\left(\frac{4J}{kT}\right) + 12 \exp\left(\frac{2J}{kT}\right) + 2}.$$

If $J = 0$, so that there was no interaction between vertices, the probability of this state would simply be $1/16$. Notice also this equation is undefined at absolute zero, $T = 0$, so its value can only be approached as a limit.

For convenience in examining the probability of this state with relation to temperature, let us set the interaction energy $J = k$. Our probability equation is now:

$$\Pr(\omega, T) = \frac{\exp\left(\frac{4}{T}\right)}{2 \exp\left(\frac{4}{T}\right) + 12 \exp\left(\frac{2}{T}\right) + 2}.$$

A graph of this probability function is shown in Figure 6.

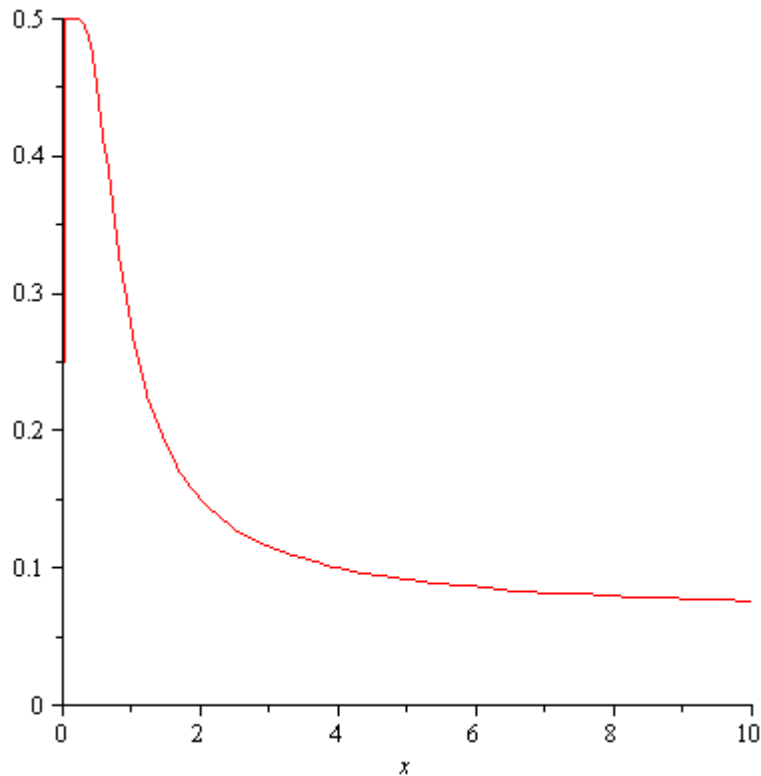


Figure 6

Notice that the probability near zero approaches fifty percent, as this is one of two lowest energy states, and that the probability approaches $1/16$ as the temperature increases.

4. TRANSFER MATRIX FORM FOR ONE DIMENSIONAL MODEL

The brute force method of summing over all possible states quickly becomes impractical with larger graphs since the number of possible states increases at a rate of 2^n (where n is the number of vertices). This limitation is partially relieved by the use of a transfer matrix formulation of the partition function. We will reformulate the partition function using a transfer matrix, and use the properties of this matrix to avoid the need to sum over every state individually. The approach here is inspired by Cibra [Cip87].

Again viewing the spins as the vectors $\langle 1,0 \rangle$ and $\langle 0,1 \rangle$, we begin by defining the transfer matrix P such that

$$\sigma_i P \sigma_j^T = \exp\left(\frac{1}{kT} J(\sigma_i \cdot \sigma_j)\right).$$

The matrix P satisfies these equations:

for like spins:

$$[1,0]P \begin{bmatrix} 1 \\ 0 \end{bmatrix} = [0,1]P \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \exp\left(\frac{J}{kT}\right).$$

and for unlike spins:

$$[1,0]P \begin{bmatrix} 0 \\ 1 \end{bmatrix} = [0,1]P \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \exp(0) = 1.$$

Thus P is a symmetric 2×2 transfer matrix which describes all possible combinations of spins between two vertices.

$$P = \begin{bmatrix} \exp\left(\frac{J}{kT}\right) & 1 \\ 1 & \exp\left(\frac{J}{kT}\right) \end{bmatrix}.$$

Using the partition function formulation described previously,

$$Z = \sum_{all \omega} \prod_{\{i,j\}} \exp\left(\frac{J}{kT} \sigma_i \cdot \sigma_j\right)$$

and the transfer matrix P , we may rewrite the partition function as

$$Z = \sum_{all \omega} \prod_{\{i,j\} \in E} \sigma_i P \sigma_j^T. \tag{1}$$

Until this point our calculations have been independent of the dimension of the graph. However, the simplifications we are about to do are only applicable to the one dimensional case of a cycle with n vertices.

With our graph a cycle of size n , we can expand Equation (1) and write:

$$Z = \sum_{\text{all } \omega} \prod_{\{i,j\} \in E} \sigma_i P \sigma_j^T = \sum_{\text{all } \omega} \sigma_1 P \sigma_2^T \sigma_2 P \sigma_3^T \sigma_3 P \sigma_4^T \dots \sigma_n P \sigma_1^T.$$

In order to format the equation for future simplification, factor the initial spin outside the summation, creating two summands; one for when the initial spin is up and one when the spin is down.

$$\begin{aligned} Z = [1,0]P & \left(\sum_{\text{all } \omega; \sigma_1=[1,0]} \sigma_2^T \sigma_2 P \sigma_3^T \sigma_3 P \sigma_4^T \dots \sigma_n P \right) \begin{bmatrix} 1 \\ 0 \end{bmatrix} \\ & + [0,1]P \left(\sum_{\text{all } \omega; \sigma_1=[0,1]} \sigma_2^T \sigma_2 P \sigma_3^T \sigma_3 P \sigma_4^T \dots \sigma_n P \right) \begin{bmatrix} 0 \\ 1 \end{bmatrix} \end{aligned} \quad (2)$$

Since for any state where the initial spin is up, there is an otherwise identical state where the spin is down, the two inner summations in this equation are equivalent.

This summation, $\sum_{\text{all } \omega; \sigma_1=[1,0]} \sigma_2^T \sigma_2 P \sigma_3^T \sigma_3 P \sigma_4^T \dots \sigma_n P$, is equal to P^{n-1} by the following induction argument:

If $n = 2$,

$$\sum_{\text{all } \omega} \prod_{i=2}^n \sigma_i^T \sigma_i P = \begin{bmatrix} 1 \\ 0 \end{bmatrix} [1,0]P + \begin{bmatrix} 0 \\ 1 \end{bmatrix} [0,1]P = P.$$

If we assume that $\sum_{\text{all } \omega} \prod_{i=2}^n \sigma_i^T \sigma_i P = P^{n-1}$ is true for some n , then this argument also holds for $n+1$ as follows.

First note that

$$\sum_{\text{all } \omega} \prod_{i=2}^{n+1} \sigma_i^T \sigma_i P = \sum_{\text{all } \omega} \left(\prod_{i=2}^n \sigma_i^T \sigma_i P \right) \cdot \sigma_{n+1}^T \sigma_{n+1} P$$

Once again we split the equation into two summands, one for an upward spin on the $n + 1^{\text{th}}$ vertex and one for a downward spin on the vertex.

$$\sum_{\text{all } \omega} \prod_{i=2}^{n+1} \sigma_i^T \sigma_i P = \left(\sum_{\text{all } \omega} \left(\prod_{i=2}^n \sigma_i^T \sigma_i P \right) \right) \begin{bmatrix} 1 \\ 0 \end{bmatrix} [1,0]P + \left(\sum_{\text{all } \omega} \left(\prod_{i=2}^n \sigma_i^T \sigma_i P \right) \right) \begin{bmatrix} 0 \\ 1 \end{bmatrix} [0,1]P$$

$$\begin{aligned}
&= \left(\sum_{\text{all } \omega} \left(\prod_{i=2}^n \sigma_i^T \sigma_i P \right) \right) \left(\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} P + \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} P \right) \\
&= \left(\sum_{\text{all } \omega} \left(\prod_{i=2}^n \sigma_i^T \sigma_i P \right) \right) P.
\end{aligned}$$

By induction, $\sum_{\text{all } \omega} (\prod_{i=2}^n \sigma_i^T \sigma_i P) = P^{n-1}$, and correspondingly,

$$\left(\sum_{\text{all } \omega} \left(\prod_{i=2}^n \sigma_i^T \sigma_i P \right) \right) P = P^{(n+1)-1} = P^n.$$

Therefore we have found for all n ,

$$\sum_{\text{all } \omega} \prod_{i=2}^n \sigma_i^T \sigma_i P = P^{n-1}$$

Returning to our partition function Z from equation (2),

$$Z = [1,0]P \left(\sum_{\text{all } \omega} \prod_{i=2}^n \sigma_i^T \sigma_i P \right) \begin{bmatrix} 1 \\ 0 \end{bmatrix} + [0,1]P \left(\sum_{\text{all } \omega} \prod_{i=2}^n \sigma_i^T \sigma_i P \right) \begin{bmatrix} 0 \\ 1 \end{bmatrix}.$$

$$Z = [1,0]P^n \begin{bmatrix} 1 \\ 0 \end{bmatrix} + [0,1]P^n \begin{bmatrix} 0 \\ 1 \end{bmatrix}.$$

The entire equation simplifies to the trace of the matrix P^n .

$$Z = \text{Tr}(P^n).$$

As the trace is simply the sum of the eigenvalues and, as for any matrix, the eigenvalues of P^n are the eigenvalues λ_1 and λ_2 of P , raised to the n th power:

$$Z = \sum_i \lambda_i^n.$$

The eigenvalues of P are $\exp \frac{J}{kT} \pm 1$, so our partition function is:

$$Z = \left(\exp \left(\frac{J}{kT} \right) + 1 \right)^n + \left(\exp \left(\frac{J}{kT} \right) - 1 \right)^n. \tag{3}$$

We now have a closed expression of the general partition function for the one dimensional Ising model on a cycle of size n .

5. PHASE TRANSITIONS ARE ABSENT IN ONE DIMENSION

The partition function is crucial to determining the existence and location of phase transitions. As stated earlier, a phase transition is a failure in analyticity as the graph becomes infinitely large which results in an abrupt change in physical properties. As magnets have a very large number of individual ions, the behavior of a magnet is best approximated by the infinite volume limit. The phase transition in ferromagnets is evident on the macro scale by a nearly instantaneous change in net magnetism.

The equations for the potential energy, kinetic energy, internal energy, specific heat, entropy, magnetism and free energy all depend on the partition function for analyticity. We will search for failure of analyticity in the function of the free energy per lattice site. Free energy is the energy available to do work. If a phase transition occurs which would require a release of latent heat to do work, this would be evident as a failure of analyticity in the free energy per lattice site. Failure of analyticity is only evident in the infinite volume limit, which is why it is crucial to solve the partition function. As the size of the cycle approaches infinity, the free energy per lattice site may be defined as

$$F = \lim_{n \rightarrow \infty} \frac{1}{n} \ln Z.$$

In the one dimensional case, using Equation (3), this becomes

$$F = \lim_{n \rightarrow \infty} \frac{1}{n} \ln \left(\left(\exp\left(\frac{J}{kT}\right) + 1 \right)^n + \left(\exp\left(\frac{J}{kT}\right) - 1 \right)^n \right).$$

We can simplify this limit by factoring $\left(\exp\left(\frac{J}{kT}\right) + 1 \right)^n$ from both terms, allowing us to split the limit into two summands.

$$F = \lim_{n \rightarrow \infty} \frac{1}{n} \ln \left(\left(\exp\left(\frac{J}{kT}\right) + 1 \right)^n \left(1 + \frac{\left(\exp\left(\frac{J}{kT}\right) - 1 \right)^n}{\left(\exp\left(\frac{J}{kT}\right) + 1 \right)^n} \right) \right)$$

$$F = \lim_{n \rightarrow \infty} \frac{1}{n} \ln \left(\exp\left(\frac{J}{kT}\right) + 1 \right)^n + \frac{1}{n} \ln \left(1 + \frac{\left(\exp\left(\frac{J}{kT}\right) - 1 \right)^n}{\left(\exp\left(\frac{J}{kT}\right) + 1 \right)^n} \right)$$

Examine the second term, $\lim_{n \rightarrow \infty} \frac{1}{n} \ln \left(1 + \left(\frac{\exp(\frac{J}{kT}) - 1}{\exp(\frac{J}{kT}) + 1} \right)^n \right)$. The value of $\exp\left(\frac{J}{kT}\right)$ is always positive, so $\left| \frac{\exp(\frac{J}{kT}) - 1}{\exp(\frac{J}{kT}) + 1} \right| < 1$, and the term $\left(\frac{\exp(\frac{J}{kT}) - 1}{\exp(\frac{J}{kT}) + 1} \right)^n$ approaches zero by the pinching theorem. Therefore we can see that $\lim_{n \rightarrow \infty} \frac{1}{n} \ln \left(1 + \left(\frac{\exp(\frac{J}{kT}) - 1}{\exp(\frac{J}{kT}) + 1} \right)^n \right) = 0$.

The free energy is dependent on the first term of our limit.

$$F = \lim_{n \rightarrow \infty} \frac{1}{n} \ln \left(\exp\left(\frac{J}{kT}\right) + 1 \right)^n.$$

$$F = \lim_{n \rightarrow \infty} \ln \left(\exp\left(\frac{J}{kT}\right) + 1 \right).$$

$$F = \ln \left(\exp\left(\frac{J}{kT}\right) + 1 \right).$$

The free energy of a site in the model is proportional to the natural logarithm of the larger eigenvalue. Thus we see that failures of analyticity in the eigenvalue indicate phase transitions. When we search for discontinuities in this equation and its derivatives, it is evident, in the one dimensional case, that there are no phase transitions since the eigenvalue (and the partition function) is fully analytical.

6. GREATER DIMENSIONALITY AND RECENT HISTORY

Ising abandoned this model soon after he discovered that the one dimensional model did not display phase transitions, as he assumed that this result would carry into higher dimensions.

However, other physicists and mathematicians pursued the model further, and it has continued to be a significant model in statistical mechanics ever since. Nearly twenty years after Ising abandoned the problem, Kramers and Wannier showed that the two dimensional model displayed phase transitions at the Curie temperature $T_c = \frac{2}{\ln(1+\sqrt{2})} \approx 2.269$ [KW41], using high and low temperature expansions of the model. In order to avoid boundary conditions, they wrapped the lattice in a corkscrew that connected to the beginning to form a torus. The partition function for two dimensions is given by:

$$Z = \sum_{\omega} \exp \left(\frac{J}{kT} \left(\sum_{\{i,j\}horizontal} \sigma_i \cdot \sigma_j \right) + \frac{J'}{kT} \left(\sum_{\{i,j\}vertical} \sigma_i \cdot \sigma_j \right) \right).$$

As this is for the general case, it is assumed that the horizontal and vertical interaction energies J and J' may be different. It was only in 1944 that this 2-dimensional partition function

was actually solved by Onsager[Ons44]. In order to avoid boundary conditions, Onsager chose to use the form of a straight torus instead of the corkscrew of Kramers and Wannier. The greatest challenge in explaining and following the analysis of the two dimensional model is the sheer number of summations and repeated operations required. In his original paper, Onsager defines four operations on spins simply to keep his equations down to a reasonable size. In the two dimensional case, the transfer matrix is infinite, representing the possibilities of a one dimensional cross section of the two dimensional model. The ingenuity of Onsager's approach is in that he does not attempt to find a partition function that applies for any size 2-dimensional model and then find its limit. Rather he begins directly with the infinite form. This allows him to focus on only one eigenvector, as the other eigenvalues fall to zero in the infinite case[Ons44].

Solving greater dimensional cases, as well as the two dimensional case with an external field, has proven extremely difficult. Noting the mathematical acrobatics Onsager managed in order to solve the two dimensional model, it is tempting to believe that with sufficient creativity and careful organizational choice the larger dimensional models can be solved. However, these larger dimension problems are NP-complete. In 1982 Barahona[Bar82] showed that the three dimensional and two dimensional with external field models are both NP-hard, as they are equivalent to finding the maximum cardinality of a stable set in a planar cubic graph, a problem known to be NP-hard[Bar82].

Istrail[Ist00] recently expanded Barahona's conclusion. He identified an underlying graph of the model, a Kuratowskian, in all non-planar varieties of the Ising model, and showed that due to the nature of this graph all non-planar varieties of the Ising model are NP-complete, regardless of whether the model itself was two or three dimensional. This conclusion applies to both the 3D Ising model and non-planar 2D models, such as the 2D model with an external field or with next-nearest neighbor interactions[Ist00]. Yet we cannot forget that it has not yet been proven that NP-complete problems are unsolvable, so the Ising model may yet be solved for larger dimensions, but an exact solution may be computationally intractable.

Nevertheless, significant work is done in specific cases of the problem, a variety of generalizations of the model, and statistical and quantum analyses of unsolved versions. The survey of [BEPS10] provides an overview of more recent applications and generalizations of the Ising model.

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